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# Incorporation of Chemical Reactions Into Building-scale Flow

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# **INCORPORATION OF CHEMICAL REACTIONS INTO BUILDING-SCALE FLOW**

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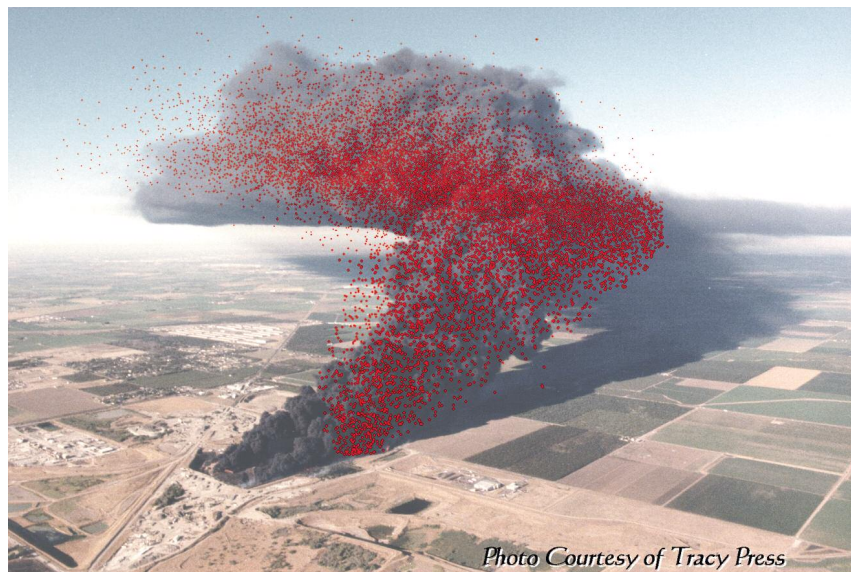
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LIVERMORE, CA**

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**Energy by the  
W-7405-Eng-48.**

# MANY ATMOSPHERIC RELEASES INVOLVE CHEMICALLY REACTING COMPOUNDS

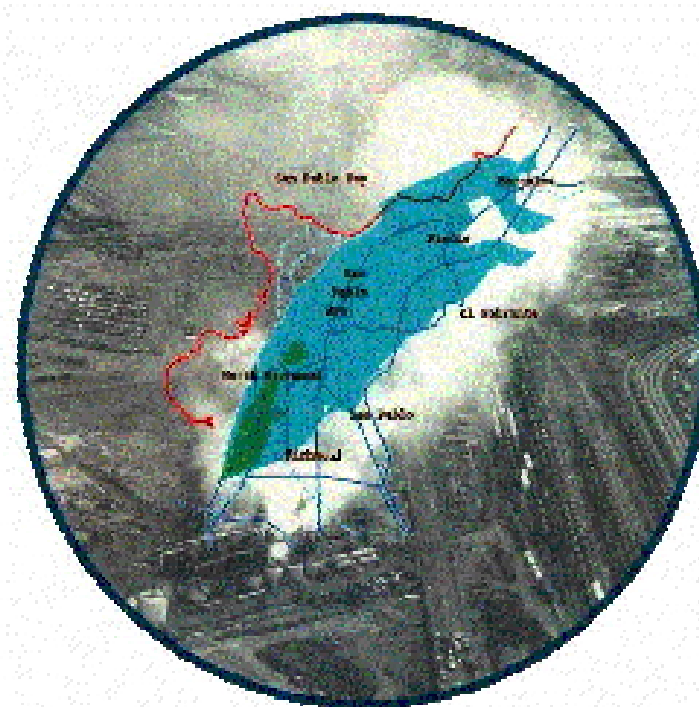


*Photo Courtesy of Tracy Press*

**1998 TRACY TIRE DUMP FIRE**



**RELEASES FROM CHEMICAL PLANTS**



**1993 RICHMOND CHEMICAL SPILL**

# Need for Chemistry and Dispersion

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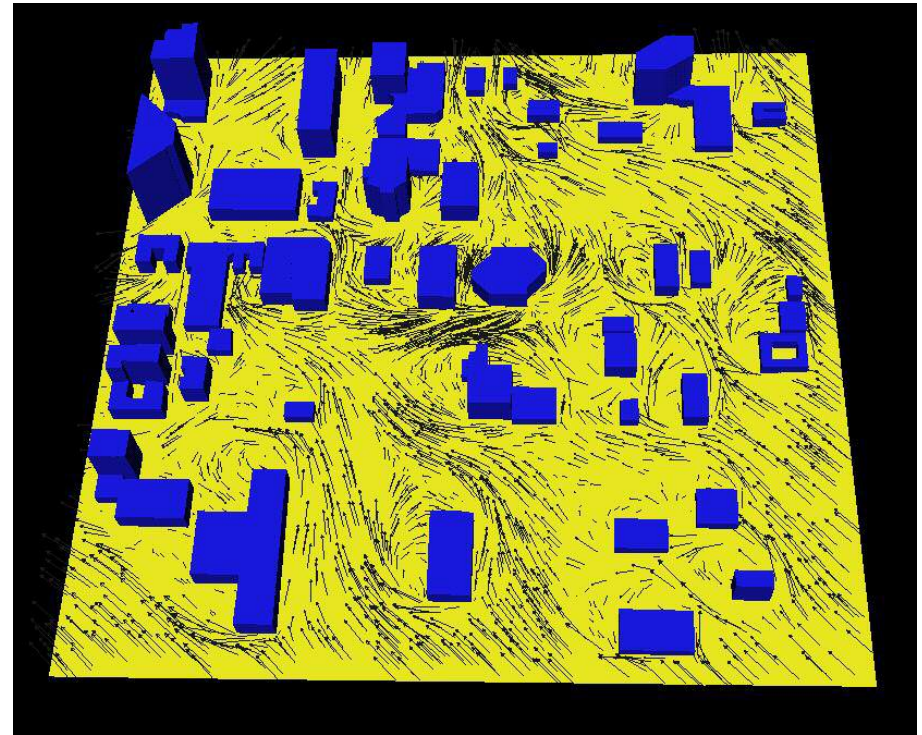
- Reactions may reduce or increase the threat posed by an atmospheric release
- Source detection depends on knowing what to look for, where
- More accurate source terms for incorporation into larger -scaled dispersion models
- Local reactant dispersion patterns resolvable with high -resolution simulations

# ComputationalFluidDynamics (CFD)Model



## FEM3MP

- FiniteElementMethod,3D, MassivelyParallel
- Subgrid ScaleModel options(e.g.,RANS,LES)
- BasicAerosolModel
- BasicSurfaceEnergy Budget
- Currentlybeingupgradedto includeAMR( Kosovic),two - wayintegrationwithlarger - scalemodels



Above:

- Domainwidth:1km
- Buildingsize:50m
- Finestgridspacing:1m
- Velocityshown:1m/sec

# ChemistryModel



## SMVGearII Solver by Mark Jacobson

- SparseMatrix, Vectorized, Gear -type integrator for first - order coupled ODE's
- Provided to us by Philip Cameron -Smith and Peter Connell (LLNL) from their global chemistry code, IMPACT

## Mechanism

- List of ~30 Species
- Reaction softype  
 $A+B \rightarrow C+D$
- Rate constants and activation energies  
Rate=
$$k * \exp(-E_a / RT) * [A] * [B]$$



# CONSTRUCTION



## Assembly

- SMVGear routines incorporated into one module of FEM3MP
- Mechanism text translated to code with scripts written by Peter Connell (LLNL)
- Mechanism code incorporated during compilation

## Testing

- Standalone SMVGear routines tested against separate box model
- FEM3MP with SMVGear routines tested with no advection or diffusion, and uniform concentrations
- Concentrations nearly independent of time step: 1 sec, 0.5 sec, 0.25 sec.

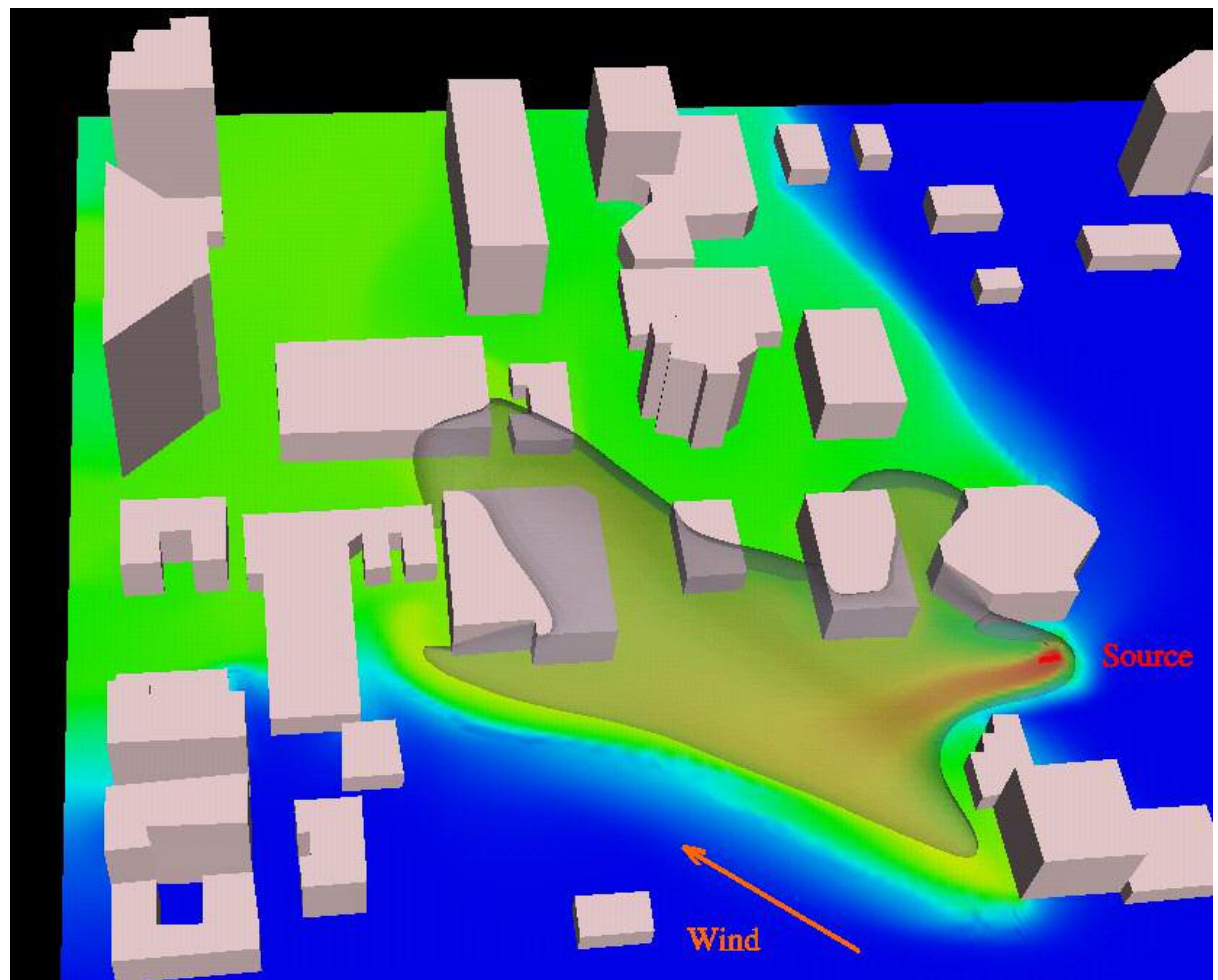


# Features of Reaction Product Plumes 1



## Limited Area of High Product Concentrations

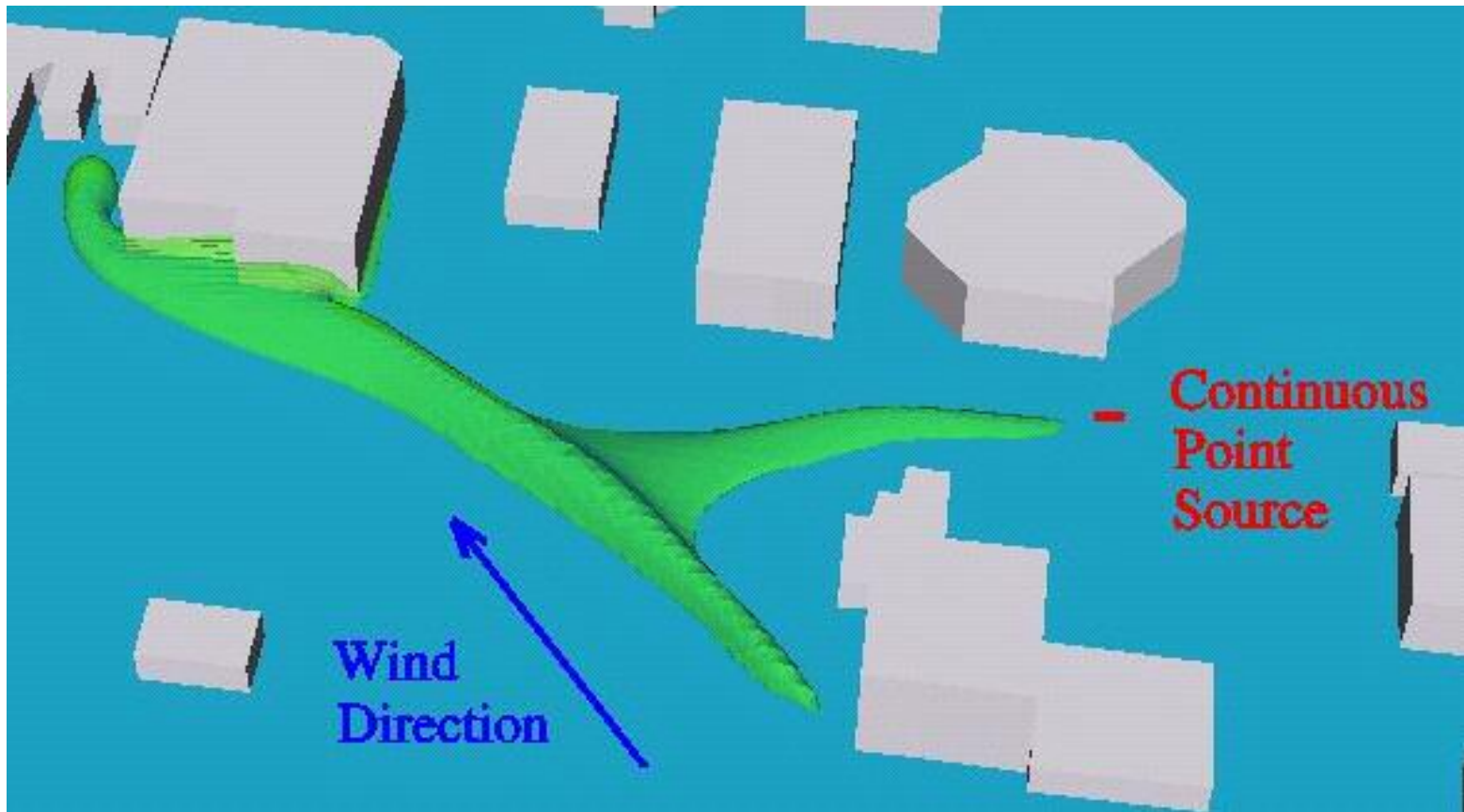
- Ground colored by release material
- Product (grey isosurface) near release only



# Features of Reaction Product Plumes 2



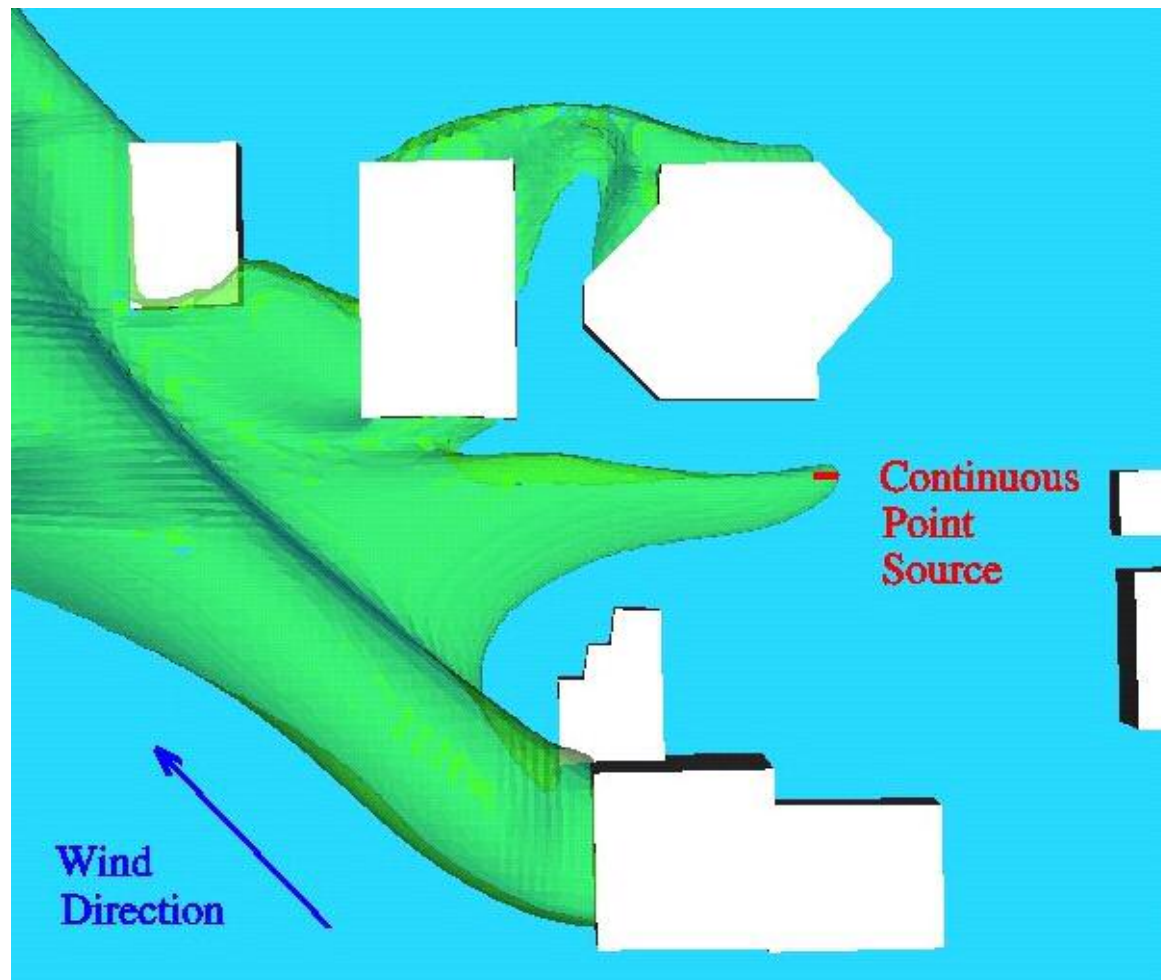
Maximum product concentration separated from source



# Features of Reaction Product Plumes 3



## Local “Hot Spots” in Building Wakes



# Current and Future Directions

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- **Include aqueous reactions within and heterogeneous reactions on the surfaces of droplets**
- **Increase number of mechanisms for common industrial and pollutant compounds**
- **Integration with larger scale chemistry models**